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TECHNIQUES FOR NUCLEAR SHIELDING CALCULATIONS

TECHNICAL DOCUMENTARY REPORT NO. ESD-TDR-63-231

May 1963

K. F. Hansen

Prepared for

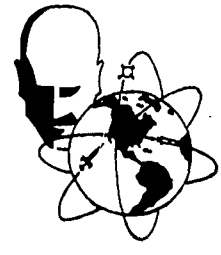
477L SYSTEM PROGRAM OFFICE

ELECTRONIC SYSTEMS DIVISION

AIR FORCE SYSTEMS COMMAND

UNITED STATES AIR FORCE

L. G. Hanscom Field, Bedford, Massachusetts



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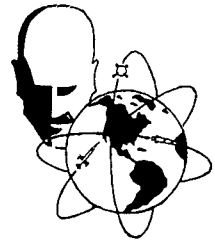

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ABSTRACT

Reviews and critiques of selected methods for nuclear shielding calculations are presented. Those techniques considered are numerical integration of the Boltzmann equation, moments method, Monte Carlo, method of successive scatterings, and removal cross-section method. An outline of the advantages and disadvantages of each particular method is included, along with a new simplified calculation procedure.

1.0 INTRODUCTION

This report consists of a review and critique of several selected methods of shielding calculations. Certain of the methods are applicable to both neutron and γ-ray penetration problems whereas others are unique for a given type of radiation. For each method outlined, a discussion of particular advantages and disadvantages is included.

The review is limited to techniques suitable for shielding studies of compact power systems. Certain methods of analysis are not considered because of their inapplicability to the problem under consideration. The shielding requirements for mobile power systems such as aircraft and rockets place a premium upon shield size and weight in contrast to stationary nuclear power plants where economics is usually the most important design parameter. The methods of shield analysis for compact power systems must be of higher order accuracy than usual since over design of the shield is undesirable. A further characteristic of shielding for mobile systems is to be noted, namely, the geometric configurations encountered will frequently lack the symmetries present in stationary plants. As always, complex geometries compound the nature of the calculational problem considerably.

The problem of reactor shielding is concerned with the biological shielding of personnel, the shielding of equipment from radiation damage, and the protection of equipment and structures from thermal damage. A complete discussion of all the problems is beyond the intent of this memorandum. However, the fundamental quantities of interest in any shielding analysis are the neutron and γ-ray flux densities as functions of position, energy, and angle. From these quantities, and certain physical parameters, all of the physical effects of radiation may be calculated. The bulk of this report will be concerned with methods of computing the neutron and γ-ray flux densities.

In the next section a brief discussion of the transport of neutrons and γ-rays is given. The third section of the report is devoted to outlining the various methods of use for shielding calculations. Section 4.0 contains a proposal for a new method of performing shielding studies. The proposal is untested for shielding calculations. The last section is a bibliography of papers, etc., giving a more general discussion of shielding theory methods.

2.0 THE TRANSPORT EQUATION FOR NEUTRONS AND PHOTONS

2.1 Neutron Transport

The basic equation of neutron conservation is the linearized Boltzmann equation. The neutron flux density, $N(\underline{r},E,\underline{\Omega})$, is defined as

$N(\underline{r},E,\underline{\Omega})$ ≡ the number of neutrons in unit volume at $\underline{r}$, within unit energy at E, within unit solid angle about $\underline{\Omega}$, which, in unit time, cross a unit element of area with normal in the direction $\underline{\Omega}$.

The statement of neutron conservation then equates losses out of a unit volume of phase space by convection and collision with gains by collision of neutrons in other elements of phase space and sources. The transport equation is then

$$\underline{\Omega} \cdot \underline{\nabla} N(\underline{r},E,\underline{\Omega}) + \sigma(\underline{r},E)\, N(\underline{r},E,\underline{\Omega}) = \int_{E'} \int_{\underline{\Omega}'} \sigma(\underline{r},E',\underline{\Omega}' \,;\, \underline{r},E,\underline{\Omega})\, N(\underline{r},E',\underline{\Omega}')\, d\underline{\Omega}'dE' + S(\underline{r},E,\underline{\Omega}) \tag{1}$$

The left-hand side gives the loss by convection and collision. $\sigma(\underline{r},E)$ is the macroscopic total cross-section and is not a function of neutron direction for isotropic media. $\sigma(\underline{r},E',\underline{\Omega}';\ \underline{r},E,\underline{\Omega})$ is the macroscopic transfer probability of neutrons from E', $\underline{\Omega}'$ to E,$\underline{\Omega}$. The transfer probability depends upon the nature of the scattering (elastic or inelastic) and the scattering law. It is convenient to consider the Boltzmann equation in terms of the lethargy variable $u \equiv \ln(E_o/E)$, where E_o is some peak energy. For fission sources, E_o is usually taken to be 15-20 Mev. For later illustrations, the transport equation for slabs will be used. For slab geometry, and in terms of the lethargy, Equation (1) is written

$$\mu \frac{d}{dx} N(x,u,\mu) + \sigma(x,u)N(x,u,\mu) = \int_{u'} \int_{-1}^{1} \sigma(x,u',\mu';\ x,u,\mu)N(x,u',\mu')\, du'd\mu' + S(x,u,\mu) \tag{2}$$

where $\mu = \cos\theta$, with θ the angle between the +x axis and the direction of neutron motion.

Various special scattering laws are easily treated. If all scattering is assumed spherically symmetric in the laboratory system, then the transfer probability is independent of μ' and μ. To first order accuracy inelastic scattering is spherically symmetric in laboratory coordinates. For elastic scattering symmetric in the center of mass system, the lethargy and scattering angle are uniquely related. Hence the integral over u' and μ' involves a δ function in one or the other variable. Note that even if the transfer probability is independent of μ', μ, the flux density is still a function of angle.

Boundary conditions for the transport equation for shielding problems are usually given in terms of incident neutrons at interfaces. Thus, for a slab shield of thickness a, adjoining a core at $x = 0$, the boundary conditions would be given at $x = 0$ for $0 \leq \mu \leq 1$. At $x = a$, assuming a vacuum boundary, the condition is $N(a,u,\mu) = 0$, $-1 \leq \mu \leq 0$. Except for rare cases, the external source is zero, or a delta function at $x = 0$ that is given by the boundary conditions.

2.2 γ-ray Transport

The transport equation for photons is the same as (1), however, simplifications are possible. The only source of scattered photons is the Compton effect(*). For Compton scattering the energy and angle are related, and again a delta function will appear in the integrand. It is convenient to change variable from the flux density to the energy density, I, where

$$I(\underline{r},E,\underline{\Omega}) = E \cdot N(\underline{r},E,\underline{\Omega})$$

In terms of I, equation (1) becomes

$$\underline{\Omega} \cdot \underline{\nabla} I(\underline{r},E,\underline{\Omega}) + \sigma(\underline{r},E)\, I(\underline{r},E,\underline{\Omega}) = \int_{E'} \int_{\underline{\Omega}'} \sigma(\underline{r},E,\underline{\Omega}';\, \underline{r},E,\underline{\Omega})\, I(\underline{r},E',\underline{\Omega}')\, \frac{E}{E'}\, dE'd\underline{\Omega}'$$

$$+ S'(\underline{r},E,\underline{\Omega}) \qquad (3)$$

If E is expressed in electron mass units, then the photon energy may be written in terms of the Compton wave length λ, with

$$\lambda = 1/E \qquad (E \text{ in electron masses})$$

(*) Other sources such as annihilation radiation and bremsstrahlung are usually negligible.

with the above change of variables, the scattering kernel is written

$$\sigma(\underline{r},E',\underline{\Omega}';\ \underline{r},E,\underline{\Omega}) = \sigma(\underline{r},\lambda',\underline{\Omega}\cdot\underline{\Omega}')\ \delta\frac{(1+\lambda'-\lambda-\underline{\Omega}\cdot\underline{\Omega}')}{E^2}$$

The scattering kernel $k(\lambda',\lambda)$ is defined as

$$k(\lambda',\lambda) = 2\pi\frac{\lambda}{\lambda'}\sigma(\lambda',\underline{\Omega}'\cdot\underline{\Omega})$$

and is given by the Klein-Nishina formula for Compton scattering. In particular,

$$k(\lambda',\lambda) = \frac{3}{8}\ \frac{\lambda'}{\lambda}\left[\frac{\lambda}{\lambda'}+\frac{\lambda'}{\lambda}+2(\lambda'-\lambda)+(\lambda'-\lambda)^2\right]\cdot A\ (\lambda' \le \lambda \le \lambda'+2)$$

$$= 0 \qquad \text{otherwise, where A is the atom density.}$$

For slabs the transport equation is thus

$$\mu\frac{d}{dx}I(x,\lambda,\mu)+\sigma(x,\lambda)\ I(x,\lambda,\mu) = \int_0^{\lambda}\int_{\underline{\Omega}'} I(x,\lambda',\mu')\ \frac{k(\lambda',\lambda)}{2\pi}$$

$$+\ \delta(1+\lambda'-\lambda-\underline{\Omega}\cdot\underline{\Omega}')\ d\underline{\Omega}'d\lambda' + S'(x,\lambda,\mu) \qquad (4)$$

The transport equation for photons is somewhat simpler than for neutrons because of the known scattering law. In particular, only photons in the wavelength range $\lambda - 2 \le \lambda' \le \lambda$ can contribute to the scattering source. This simplification of the scattering source is particularly useful in numerical integration and moments expansions of the transport equation for photons.

3.0 SELECTED METHODS OF SHIELD CALCULATIONS

In view of the complex nature of the Boltzmann equation analytic solutions are possible only for the simplest of problems. A number of procedures for approximate shield calculations have been proposed. All of the methods represent approximations to the transport equation, either numerical approximations, or simplifying physical approximations. Several methods of both types will be considered.

3.1 Numerical Integration of the Boltzmann Equation

There are numerous numerical approximations used for transport calculations. Rather than outline a particular method, such as the S_N method, a general procedure is considered. The approach is sufficient to indicate the nature of the approximations inherent in the method.

Basically every numerical approximation is found by dividing continuous variables into discrete variables and solving the resultant difference equations. Values intermediate to the discrete points are found by interpolation. For the transport problem, for neutrons, the lethargy, angle, and spatial ranges are discretized. First the lethargy interval $0 \leq U \leq U_{th}$ is divided into G groups, not necessarily of equal spacing, with $\Delta U_g \equiv \Delta_g = U_g - U_{g-1}$. A thermal group with index G+1 is appended. Integration of the Boltzmann equation (2) over the interval Δ_g yields

$$\mu \frac{d}{dx} \overline{N^g}(x,\mu) + \overline{\sigma^g}(x,\mu)\, \overline{N^g}(x,\mu) = \int_{u_{g-1}}^{u_g} du \left[\int_{u'}^{1} \int_{-1}^{1} \sigma(x,u',\mu';\, x,u,\mu)\, N(x,u',\mu') \right.$$

$$\left. du'd\mu' \right] + \overline{S^g}(x,\mu) \qquad (5)$$

The quantities $\overline{N^g}$, $\overline{\sigma^g}$, $\overline{S^g}$ denote average values of the variable in the interval Δ_g. Thus,

$$\overline{N^g}(x,\mu) = \frac{1}{\Delta_g} \int_{u_{g-1}}^{u_g} N(x,u',\mu)\, du'$$

and

$$\overline{\sigma^g}(x,\mu) = \frac{\int_{u_{g-1}}^{u_g} \sigma(x,u')\, N(x,u',\mu)\, du'}{\int_{u_{g-1}}^{u_g} N(x,u',\mu)\, du'}$$

Note that although $\sigma(x,u)$ is not a function of μ, the average value of the cross-section, $\overline{\sigma^g}$, is a function of μ. Usually the variation of $\overline{\sigma^g}$ with μ is ignored since $N(x,u,\mu)$ is a reasonably flat function of μ for reactor calculations. In shield calculations there may be a very highly anisotropic flux distribution, particularly at deep penetrations and high energies, in which case the distinction is important.

An immediate difficulty with the numerical procedure is apparent. The proper cross-sections for the group equations cannot be computed until the solution is known. In reactor calculations the properly weighted cross-sections are frequently found by assuming a spectrum initially or by computing on approximate spectrums from an infinite medium calculation. The infinite medium method is useful for shield calculations where the spectrum "hardening" with increasing depth may be explicitly included.

Assuming that properly weighted coefficients may be found then the scattering integral can be handled. The integration over u' is approximated by a sum, such as

$$\int_{-1}^{1} \int_{u_{g-1}}^{u_g} \int_{u'} \sigma(x,u',\mu';\ x,u,\mu)\ N(x,u',\mu')\ du' = \int_{-1}^{1} d\mu' \sum_{g'=1}^{G+1} \overline{\sigma^{g',g}}(x,\mu';x,\mu)\overline{N^{g'}}(x,\mu') \tag{6}$$

where $\overline{\sigma^{g',g}}$ represents the transfer probability from group g' to group g. The determination of, $\overline{\sigma^{g',g}}$ depends upon the scattering law and the weighting function used for the lethargy integration. The sum includes all of the groups. For shielding purposes the thermal region is rarely divided into many groups, hence shield calculations characteristically contain fewer groups than criticality calculations. In general, low energy neutrons are rapidly absorbed and do not up-scatter. In this case, all elements of $\overline{\sigma^{g',g}}$ are zero for $g' > g$. For elastic scattering only elements for g' near g are non-zero. For inelastic scattering g' may be far removed from g.

The angular variation is treated in similar fashion. The range $-1 \le \mu \le 1$ is divided into segments of width $\Delta\mu_n \equiv \Delta_n = \mu_n - \mu_{n-1}$. The various terms in the group transport equation (5) may be integrated over Δ_n as before. The integration yields

$$\int_{\mu_{n-1}}^{\mu_n} \mu \frac{d}{dx} \overline{N^g}(x,\mu)\ d\mu \approx \alpha_n \frac{d}{dx}\left[\overline{N_n^g}(x) + \overline{N_{n-1}^g}(x)\right]$$

$$\int_{\mu_{n-1}}^{u_n} \overline{\sigma^g}(x,\mu)\ \overline{N^g}(x,\mu)\ d\mu = \beta_n \left[\overline{N_n^g}(x) + \overline{N_{n-1}^g}(x)\right]$$

where α_n, β_n are weight coefficients which depend upon the quadrature rule assumed. For instance, in the S_n method $\overline{N^g}(x,\mu)$ is assumed to vary linearly over an interval. For the Wick method, the gaussian weight functions are used. Obviously many different possibilities exist.

The transfer probabilities from equation (6) may be written

$$\int_{\mu_{n-1}}^{\mu_n} d\mu \int_{-1}^{1} d\mu' \left[\sum_{g'} \overline{\sigma^{g',g}}\,(x,\mu';\, x,\mu)\; \overline{N^g}(x,\mu') \right] d\mu' = \sum_{n'} \sum_{g'} \overline{\sigma_{n',n}^{g',g}}(x)\; \overline{N_{n'}^{g'}}(x)$$

The group transport equation is then of the form

$$\alpha_n \frac{d}{dx}\left[\overline{N_n^{\,g}}(x) + \overline{N_{n-1}^{\,g}}(x)\right] + \beta_n\left[\overline{N_n^{\,g}}(x) + \overline{N_{n-1}^{\,g}}(x)\right] = \sum_{n'} \sum_{g'} \overline{\sigma_{n',n}^{g',g}}(x)\; \overline{N_{n'}^{\,g'}}(x)$$

$$+ S_n^{\,g}(x) \tag{8}$$

The spatial variation is treated as before. In general the result is a difference equation coupling various mesh points in the indices g,n,j (j is a spatial index). A typical difference equation would be of the form

$$r_{n,j}\, N_{n,j}^{\,g} + l_{n,j}\, N_{n,j-1}^{\,g} + t_{n,j}\, N_{n-1,j}^{\,g} + b_{n,j}\, N_{n-1,j-1}^{\,g} =$$

$$\sum_{n',g'} T_{n',n;j}^{\,g',g}\, N_{n',j}^{\,g'} + S_{n,j}^{\,g} \tag{9}$$

$$g = 1,2, \ldots, G+1$$
$$n = 0,1, \ldots, N$$
$$j = 0,1, \ldots, J$$

The result is a very large set of simultaneous algebraic equations.

The method of solution is straight forward. An initial distribution, consistent with the boundary conditions, is assumed. The difference relation (9) is applied repetitively to each point until a convergent solution is obtained. Further comments on the solution of algebraic equations are given in Section 4.0.

From the elementary sketch above, it is possible to assess the advantages and disadvantages of the direct integration method. The advantages are several:

1) Inhomogeneous media and finite media are readily incorporated into the analysis.

2) Complex scattering kernels can be approximated by the transfer matrix $\sigma_{n',n}^{g',g}$.

3) The truncation error associated with discretizing can be reduced by refinement of the mesh.

4) The method yields all of the desired information, i.e., $N(r,u,\mu)$.

5) The results are not subject to statistical variation, hence the method is readily adapted for deep penetrations.

6) Surveys may be made rapidly by reducing the number of discrete variables.

The disadvantages associated with the method are rather severe.

1) For detailed studies the amount of machine time is very large. In particular, the number of iterations to reach a solution is roughly proportional to the square of the unknowns. To double the mesh size in each dimension increases the computation time by a factor of 64 approximately.

2) Higher dimension problems, and irregular geometries, increase the computational burden. Two and three space dimension problems are at the limit of present machine capabilities.

3) The proper weighted cross-sections are difficult to find and require a subsidiary calculation of the same order of magnitude as the original problem.

4) Reduction of truncation error increases the computational time in roughly quadratic fashion.

3.2 The Moments Method

The basis of the moments method is an expansion of the angular and spatial dependence of the flux density. The objective of the expansion is to decouple the complex behavior of the flux density into a set of variables which may be recombined to approximate the flux density. The

expansion should be carried out in such a manner that the resulting simultaneous equations for the expansion variables are easy to solve, and further, the expansion variables should form a rapidly convergent sequence.

The process of reduction is outlined for a plane problem for photons. The transport equation is

$$\mu \frac{d}{dx} I(x,\lambda,\mu) + \sigma(x,\lambda)\ I(x,\lambda,\mu) = \int_0^{\lambda} \int_{\underline{\Omega}'} I(x,\lambda',\mu')\ k(\lambda',\lambda) * \\ * \frac{\delta(1 + \lambda' - \lambda - \underline{\Omega} \cdot \underline{\Omega}')}{2\pi}\ d\underline{\Omega}' d\lambda' + S(x,\lambda,\mu). \tag{10}$$

The expansion for the angular coordinates is in terms of the Legendre polynomials $P_\ell(\mu)$ whereas the spatial expansion is in terms of the spatial moments moments x^n. The generalized moment, say $b_{n,\ell}(\lambda)$, is determined as

$$b_{n,\ell}(\lambda) = \frac{2\pi\sigma_0^{n+1}}{n!} \int_{-\infty}^{\infty} dx \int_{-1}^{1} d\mu P_\ell(\mu) x^n I(x,\lambda,\mu) \tag{11}$$

where σ_0 is the cross-section at the largest source energy. The choice of constants facilitates normalization.

The objective is to reduce the transport equation to coupled equations (through n and ℓ) for the variable $b_{n,\ell}(\lambda)$.

The first step in the reduction of the transport equation is to carry out the angular expansion. The expansion

$$I(x,\lambda,\mu) = \sum_{\ell} \frac{2\ell + 1}{4\pi} I\ (x,\lambda)\ P_\ell(\mu)$$

is used. By the orthogonality of the $P_\ell(\mu)$

$$I_\ell(x,\lambda) = 2\pi \int_{-1}^{1} I(x,\lambda,\mu)\ P_\ell(\mu) d\mu$$

By multiplying equation (10) by $P_\ell(\mu)$ and integrating over all $\underline{\Omega}$ we have

$$\frac{\ell+1}{2\ell+1}\frac{dI_{\ell+1}}{dx} + \frac{\ell}{2\ell+1}\frac{dI_{\ell-1}}{dx} + \sigma(x,\lambda)I_\ell = \int_0^\lambda P_\ell(1+\lambda'-\lambda)\, k(\lambda',\lambda) *$$

$$I_\ell(x,\lambda')\, d\lambda' + S_\ell(x,\lambda) \qquad (12)$$

The proof of (12) follows from the addition theorem for Legendre polynomials and the known recursion relations for the $P_\ell(\mu)$. Equation (12) applies for $\ell = 0,1,2, \ldots$.

The spatial dependence is eliminated from the definition (11), that is

$$b_{n,\ell}(\lambda) = \frac{\sigma_o^{n+1}}{n!}\int_{-\infty}^{\infty} I_\ell(x,\lambda)\, x^n dx$$

To find the equation for the $b_{n,\ell}(\lambda)$ we multiply (12) by $\frac{\mu_o^{n+1}}{n!}x^n$ and integrate over all x. The left-hand side is considered first. The derivative terms are integrated by parts to yield

$$\frac{\ell+1}{2\ell+1}\frac{\sigma_o^{n+1}}{n!}\left\{ x^n I_{\ell+1}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} nx^{n-1} I_{\ell+1}(x,\lambda)dx \right\} + \frac{\ell}{2\ell+1}\frac{\sigma_o^{n+1}}{n!}\left\{x^n I_{\ell-1}\Big|_{-\infty}^{\infty}\right.$$

$$\left. - \int_{-\infty}^{\infty} nx^{n-1} I_{\ell-1}(x,\lambda)dx\right\} + \frac{\sigma_o^{n+1}}{n!}\int_{-\infty}^{\infty}\sigma(x,\lambda)I_\ell(x,\lambda)dx \qquad (13)$$

In order for the integrated terms to vanish, it is necessary that I_ℓ vanish faster than x^n for large x. An immediate consequence of this restriction is that the medium must be infinitely thick. Obviously this represents a serious restriction. Equally important is that fact that $\sigma(x,\lambda)$ must actually be independent of x, and thus the moments method only applies to homogeneous media. The above two restrictions limit the applicability of the method particularly to compact power systems.

With the above assumptions, equation (13) becomes

$$\sigma(\lambda)\, b_{n,\ell}(\lambda) - \sigma_o\left\{\frac{\ell+1}{2\ell+1} b_{n-1,\ell+1}(\lambda) + \frac{\ell}{2\ell+1} b_{n-1,\ell-1}(\lambda)\right\} \qquad (14)$$

The right-hand side of equation (12) is easily found to be

$$\int_0^{\lambda} P_\ell(1 + \lambda' - \lambda)\ k(\lambda',\lambda)\ b_{n,\ell}(\lambda')d\lambda' + S_{n,\ell}(\lambda)$$

The Boltzmann equation reduces to

$$\sigma(\lambda)\ b_{n,\ell}(\lambda) = \int_0^{\lambda} P_\ell(1 + \lambda' - \lambda)\ k(\lambda',\lambda)\ b_{n,\ell}(\lambda')d\lambda' +$$

$$\sigma_o \left\{\frac{\ell+1}{2\ell+1}\ b_{n-1,\ell+1}(\lambda) + \frac{\ell}{2\ell+1}\ b_{n-1,\ell-1}(\lambda)\right\} + S_{n,\ell}(\lambda) \qquad (15)$$

The aim of the method has been achieved in that a coupled set of simple equations have been found for the moments of the expansion. The integral is evaluated numerically since the functions $P_\ell(\lambda',\lambda)$ and $k(\lambda',\lambda)$ are known. Further, the integration is over the range $\lambda - 2 \le \lambda' \le \lambda$ and hence the entire integrand is known.

For the case of neutron penetration, the integration is more involved since the range of integration is from $0 \le u \le u'$, and furthermore, the scattering kernel is not as simple a function as for γ-rays. For neutrons an approximate kernel is derived in a manner similar to the methods of direct numerical integration.

The equation for the moments, (15), is solved sequentially for $n = 1, 2 \ldots$. Note that the equation couples only lower moments together and hence no truncation is necessary to solve for any given moment. This is in contradistinction to the usual spherical harmonics method of neutron transport.

The reconstruction of the energy density is reasonably straight forward. It is sufficient to find the coefficients $I_\ell(x,\lambda)$. The objective is to find a rapidly convergent expansion for the function $I_\ell(x,\lambda)$. The coefficients $b_{n,\ell}(\lambda)$ are not directly useful since the factors x^n do not obey a simple orthogonality rule. The following physical approximation is usually applied. The behavior of the flux density with increasing penetration is roughly exponential. An expansion of the form

$$I_\ell(x,\lambda) = \sum_n a_{n,\ell}(\lambda)\ e^{-\sigma_o x}\ p_n(x) \qquad (16)$$

with $p_n(x)$ a polynomial of degree n, is assumed. The coefficients can be evaluated as

$$a_{n,\ell}(\lambda) = \int_{-\infty}^{\infty} I_{\ell}(x,\lambda)p_n(x) \tag{17}$$

if the $p_n(x)$ are the Laguerre polynomials. But from the definition of $b_{n,\ell}(\lambda)$, the $a_{n,\ell}(\lambda)$ are linear combinations of the $b_{n',\ell}(\lambda)$ for $n' = 1,2, \ldots, n$. That is,

$$a_{n,\ell}(\lambda) = \sum_{n'} c_{n'} b_{n',\ell}(\lambda). \tag{18}$$

Several points are worth noting. First, the expansion (16) was particularly chosen so that the coefficients were easily found, as by equation (17). Obviously other weight functions than $e^{-\sigma_o x}$ are possible. Different weight functions give different coefficients, but orthogonality relations relative to a weight function are readily found. The choice of $e^{-\sigma_o x}$ is particularly useful since only a few $a_{n,\ell}(\lambda)$ are needed, i.e., the series converges rapidly.

The Boltzmann equation could have been expanded directly in terms of the $a_{n,\ell}(\lambda)$ instead of the $b_{n,\ell}(\lambda)$. In a certain sense the $b_{n,\ell}(\lambda)$ are more general in that the appropriate coefficients for weight functions other than unity are most readily obtained from the $b_{n,\ell}(\lambda)$. Thus the $b_{n,\ell}(\lambda)$ are the simplest to use for finding expressions such as (18).

The basic elements of the moments method are now clear. The calculational procedure is simple (particularly for photons) and the reconstruction of the flux density allows wide latitude for use with rather involved weight functions. The development does illustrate the particular advantages and disadvantages of the method.

Advantageous properties of the method include

1) The method yields quite accurate results for deep penetrations.
2) Relatively universal penetration curves can be derived and used to study composite media without additional calculation.
3) Machine time is relatively small compared to direct integration.
4) The method lends itself readily to deriving elementary equations which approximate the solution.
5) Ancillary information such as build-up factors are easily found.

The disadvantages are quite serious for compact shields.

1) The requirement of an infinite medium. By use of approximate formulas this restriction can be made less severe.
2) Homogeneous media. This is very serious and not removable.
3) The determination of the angular distribution requires many approximations since the proper weight functions in the expansions are not readily apparent.
4) The results are generally applicable only beyond several mean free paths, thus the full flux density is not found.
5) In many cases the accuracy of the result is hard to determine.

3.3 The Monte Carlo Method

The Monte Carlo method is a statistical sampling procedure for conducting theoretical experiments on particle distributions. In its simplest form the method consists of a straightforward calculation of many particle histories. The results yield a probabilistic measure of the penetration and distribution of particles. Usually a straightforward reproduction of histories is inefficient and a variety of modifications to the procedure are adopted to yield equivalent results with less effort.

The basis of Monte Carlo calculations is the Central Limit Theorem of Statistics. The theorem relates theoretical first and second moments of distribution functions to the normal distribution. Let $f(x)$ denote a distribution function, hence

$$\int_{-\infty}^{\infty} f(x)\,dx = 1$$

The first moment of the distribution, the mean value, is then

$$\langle x \rangle = \int_{-\infty}^{\infty} x f(x)\,dx$$

The second moment is

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 f(x)\,dx$$

A very useful statistical quantity is the second moment about the mean, usually called the variance r. Evidently

$$r = \langle (x - \langle x \rangle)^2 \rangle = \int_{-\infty}^{\infty} (x^2 - 2x\langle x \rangle + \langle x \rangle^2)\, f(x)\,dx$$

$$= \langle x^2 \rangle - \langle x \rangle^2$$

The square root of the variance is called the standard deviation and denoted

$$\sigma = \sqrt{r}$$

The Central Limit Theorem then states that if a finite number of values of x, say x_i, $1 \leq i \leq N$,

$$\bar{x} = \frac{1}{N} \sum_i x_i$$

Then the variable $\frac{\bar{x} - \langle x \rangle}{\frac{\sigma}{\sqrt{N}}}$ has a distribution that approaches a normal distribution for large N. In other words

$$\bar{x} \approx \langle x \rangle$$

with an approximately normal distribution with standard deviation

$$\bar{\sigma} = \frac{\sigma}{\sqrt{N}}$$

The approach to the normal distribution is accurate to terms $0(1/\sqrt{N})$ which is negligible for large N.

The importance of the Central Limit Theorem is apparent, since it is then possible to evaluate the mean of a distribution and to find the limits of confidence on the calculated value. This is precisely the problem the Monte Carlo is addressed to.

Generalizations of the Central Limit Theorem are readily found. Thus, if g(x) is some function of x, where x is distributed according to the distribution f(x) then

$$\langle g \rangle = \int_{-\infty}^{\infty} g(x) f(x) dx$$

and

$$\langle g^2 \rangle = \int_{-\infty}^{\infty} g^2(x) f(x) dx$$

and

$$r_g = \langle g^2 \rangle - \langle g \rangle^2$$

The Central Limit Theorem is then

$$\bar{g} = \frac{1}{N} \sum_i g(x_i) \approx \langle g \rangle$$

$$\bar{\sigma}_g = \frac{\sigma_g}{\sqrt{N}} = \sqrt{\frac{\langle g^2 \rangle - \langle g \rangle^2}{N}}$$

In most cases the Monte Carlo method is used to find $\bar{g}$ with σ_g not known. A statistical estimate of σ_g may be found readily. The expected value of $\bar{g}$ is

$$\langle \bar{g} \rangle = \int_{-\infty}^{\infty} \frac{1}{N} \sum_i g(x_i) f(x) dx = \frac{1}{N} \left[\sum_i \langle g \rangle \right] = \langle g \rangle$$

that is the expected value of $\bar{g}$ is the mean. Hence $\bar{g}$ is an unbiased estimate of $\langle g \rangle$. The expected value of the sample variance $\overline{g^2} - \bar{g}^2$ is

$$\langle \overline{g^2} - \bar{g}^2 \rangle = \frac{1}{N} \int_{-\infty}^{\infty} \sum_i (g(x_i) - \bar{g})^2 f(x) dx$$

$$= \frac{1}{N} \sum_i \int_{-\infty}^{\infty} f(x) dx \left[(g(x_i) - \langle g \rangle)^2 - (\bar{g} - \langle g \rangle)^2 \right]$$

$$= \frac{1}{N}\sum_{i}\left[\sigma_g^{\,2} - \overline{\sigma_g}^{\,2}\right] = \sigma_g^{\,2} - \frac{\sigma_g^{\,2}}{N}$$

$$\therefore \sigma_g^{\,2} = \frac{N}{N-1}\left[\overline{g^2} - \overline{g}^2\right]$$

Thus,

$$\overline{\sigma_g} = \sqrt{\frac{\overline{g^2} - \overline{g}^2}{N-1}}$$

Hence a statistical estimate of the standard deviation for the distribution of $\overline{g}$ is readily available.

The two central problems of the Monte Carlo method are seen to be:

1) Selection of x_i from a distribution $f(x)$
2) Reduction of the sample variance

The selection from a distribution function is usually accomplished by use of random numbers, i.e., numbers distributed uniformly in the interval $0 \le \xi \le 1$. If the cumulative distribution $F(x)$ is defined as

$$F(x) = \int_{-\infty}^{x} f(x)\,dx$$

and if a random number ξ is chosen then

$$x = F^{-1}(\xi)$$

is a random variable x selected from $f(x)$. This follows since

$$\xi = F(x)$$

and

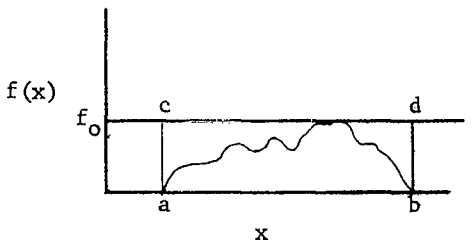
$$p(\xi)\,d\xi = p(x)\,dx$$

Since $p(\xi) = 1$ we have

$$p(x) = \frac{d\xi}{dx} = f(x)$$

hence x distributed according to f(x)

For multi-dimensional and complicated distributions direct evaluation may be impractical and the rejection technique is often used. The method is illustrated for a one dimensional distribution f(x). If f(x) has the distribution as shown below



where the limits are $a \leq x \leq b$ and $f_o = \max f(x)$, then the rectangle abcd contains all of f(x). Two random numbers ξ_1, ξ_2 are used to determine a point in the rectangle. If (ξ_1, ξ_2) lies within f(x) then ξ_1 is accepted, otherwise the process is repeated. The geometric interpretation of the method is evident.

There are many other methods of selection which are not enumerated here.

The reduction of sample variance may obviously be achieved by increasing the number of samples N. Alternate methods are to modify the sampling probabilities to decrease the sample variance $\overline{g^2} - \bar{g}^2$. Particularly useful techniques are considered for the penetration problem.

Let p denote the probability of a particle penetrating the shield and (1-p) the probability of not penetrating. If N particles are incident, then the probability of S penetrating is

$$P_S = \frac{N!}{S!(N-S)!} \; p^S (1-p)^{N-S}$$

i.e., a binomial distribution. The mean of the distribution is Np and the variance Np(1-p). The fraction transmitted is $\frac{\langle s \rangle}{N} = p$, with variance $\frac{p(1-p)}{N}$. The error in the estimated value of p, say e, is

$$e \alpha \sqrt{\frac{p(1-p)}{N}}$$

and the fractional error is

$$\frac{e}{p} \alpha \sqrt{\frac{(1-p)}{Np}} \tag{19}$$

Obviously for small p the fractional error will be small only for large N.

To reduce the error, i.e., the sample variance, it is frequently possible to modify the penetration probability in a known manner such that the new penetration probability, say p', is greater than p. In particular, if p' can be made equal to unity then the error is zero and p can be determined exactly. Note that the transformation from p to p' must be known so that p may be computed from the estimated p'. An alternative procedure is to modify the calculation procedure such that the correct p is estimated but the sample variance of the procedure is different from (19), and hopefully smaller. Examples of both types of reduction of variance will be shown.

The increase of penetration probability may be achieved by the exponential transformation. The transformation is best understood by reference to the Boltzmann equation in the form

$$\mu \frac{dI}{dx} + \sigma I = F(x,\lambda,\mu)$$

The spatial variation of I(x) is of the form

$$I(x) = e^{-\frac{\sigma}{\mu}x} \left[G(x,\lambda,\mu) \right]$$

For straight ahead particles, i.e., $\mu = 1$, the penetration is roughly proportional of $e^{-\sigma x}$. For thick shields the probability of penetration is very small. To increase the penetration probability the transformed variable

$$\bar{I}(x,\lambda,\mu) = e^{\alpha x} I(x,\lambda,\mu)$$

is considered. In terms of the transformed variable the Boltzmann equation is

$$\mu \frac{d}{dx} \bar{I} + (\sigma - \alpha) \bar{I} = F'(x,\lambda,\mu)$$

and hence the attenuation factor may be reduced by proper choice of α. Usually α is slightly smaller than the minimum of σ. The Monte Carlo evaluation of $\bar{I}$ yields an estimate p' with small fractional error. p is then merely $e^{-\alpha x}p'$ with the same fractional error.

Other variance reduction schemes can be used with yield the same p, but different variance. A particularly notable method is the importance-sampling technique. As applied to penetration problems the basis of the method is the following. When a particle is heading out of the shield it is "important" to follow the particle since it may penetrate. Conversely, a particle heading back into the shield has a smaller chance of penetrating and hence is less important. It is advantageous to bias the particle behavior so that collisions favor forward scattering of the particle at the expense of back-scattering. Thus the probability of forward scatter might be made n times more likely than back-scatter. To eliminate the bias introduced, the forward scattered particle is not counted as one particle but 1/nth of a particle. The result of the sampling procedure is that most of the computation time is spent treating forward moving particles.

Extensions of the method are readily available. Since the bias scattering introduces a "weight" associated with particles we may use other weighting procedures. For instance, instead of terminating a particle history by absorption, we might reduce the particle weight by σ_a/σ_t at each collision and make all collisions scatterings. In this case, no particle dies by collision but only when the weight gets too small to contribute sensibly to the penetration.

A further extension of the same basic procedure is the "Splitting and Russian Roulette" procedure. In this method one emphasizes deep penetration by splitting each particle that penetrates to a given depth into several particles of reduced weight. If a particle returns toward the source then a subsidiary game of Russian roulette is played, where the particles chance of survival is equal to the reduced weight of the splitting. Usually several splitting planes are introduced at various depths.

Another process of using weights is the use of expected values. Suppose a particle is at point x heading in the direction of μ. The probability of penetration, without further collision is calculable as

$$W_o = e^{-\frac{\sigma}{\mu}(T-x)}$$

with T the shield thickness. An amount of penetration W_o is tallied and the particle is given the reduced weight $(1 - W_o)$. The particle is then followed until a collision occurs or the particle penetrates. If the particle penetrated the score $(1 - W_o)$ is tallied and a new particle studied. If a collision occurs the new energy and direction parameters

are determined (and perhaps a new weight). Let the resulting particle have a weight $\alpha_1(1 - W_o)$. The penetration without further interaction is W_1. The score $W_1 \alpha_1 (1 - W_o)$ is tallied and the remaining particle is given the weight $\alpha_1(1 - W_o)(1 - W_1)$. The process continues until the weight becomes negligible or the particle penetrates.

Occasionally a particle with very small weight reaches a very important region of the problem - for instance very near the edge of the shield. In such a case, the particle need not be killed because of the low weight, but may be given a chance to survive by the Russian roulette game. If the particle survives the Russian roulette, the weight is increased accordingly. This procedure is obviously a combination of importance sampling and Russian roulette.

The estimated statistical variance when using any or all of the above methods is frequently difficult to ascertain. For some rather classical problems (evaluation of integrals) the estimated variance reduction is more easily found.

The evaluation of the Monte Carlo method is given below.

Advantages:

1) The method is useful for highly inhomogeneous media and for irregular and/or higher dimension geometries.

2) It is possible to study perturbations directly rather than consider two separate problems.

3) By appropriate choice of the method of analysis any given property of the shield can be studied, for instance, reflection coefficients rather than transmission.

4) With a proper selection of variance reduction, the computational time may be much smaller than direct integration and/or the moments method.

5) Very complicated interaction probabilities are readily incorporated into the collision mechanics without approximation.

Disadvantages:

1) Frequent lack of reliable error estimates.

2) Results may be seriously in error without any statistical indication available.

Disadvantages, Cont.:

3) For some problems the time of computation may be excessive - this is usually true for problems of small asymmetry and few dimensions.

4) Distribution functions to be sampled may be very complex and time consuming to select from

5) Problem must usually be designed to yield only limited data due to time and storage problems.

3.4 Method of Successive Scatterings

The method of successive scatterings was developed for γ-ray penetration problems, particularly in slab geometry. The technique has the virtue of being applicable to multi-layer shields. Further, the method is only used for finite shields which may have any desired thickness.

The basis of the method is to consider the fractional transmission of photons of 0, 1, . . . k scatterings within the shield. If $N_k(a,\lambda_o,\mu_o)$ is the fraction of the incident photons transmitted which undergo k collisions, then

$$N(a,\lambda_o,\mu_o) = \sum_{k}^{\leftarrow} N_k(a,\lambda_o,\mu_o)$$

where N is the total fraction transmitted. The difficult part of the method is the determination of the N_k $k > 0$. For $k = 0$, we have

$$N_o(a, \lambda_o,\mu_o) = e^{-\frac{\sigma_o a}{\mu_o}}$$

The factor N_1 can be found as follows. N_1 consists of all photons which undergo a first collision and then escape. The probability of traveling a distance x into the shield is merely

$$e^{-\frac{\sigma_o x}{\mu_o}}$$

The probability of undergoing a collision within dx is $\sigma_o \frac{dx}{\mu_o}$. The probability of scattering through the angle θ with respect to the initial direction is

$$\frac{\sigma_s(\theta,\lambda_o)\,d\Omega}{\sigma_o}$$

Finally, the probability of being transmitted without further collision is $N_o(a - x,\lambda,\mu)$ where λ is the wavelength of the scattered photon and μ the direction cosine. Thus,

$$dN_1 = e^{-\frac{\sigma_o x}{\mu_o}} \frac{\sigma_o dx}{\mu_o} \frac{\sigma_s(\theta,\lambda_o)\ d\Omega\ N_o(a-x,\lambda,\mu)}{\sigma_o}$$

or

$$N_1(a,\lambda_o,\mu_o) = \int_o^a dx \int_\Omega d\Omega \frac{e^{-\frac{\sigma_o x}{\mu_o}}}{\mu_o} \sigma_s(\theta,\lambda_o)\ N_o(a-x,\lambda,\mu) \tag{20}$$

The only elements of the integral over the solid angle which can contribute to the transmission are those for which θ such that $\mu > 0$. We then have

$$N_1(a,\lambda_o,\mu_o) = \int_o^a dx \int_{\mu>0} d\Omega \frac{e^{-\frac{\sigma_o x}{\mu_o}}}{\mu_o} \sigma_s(\theta,\lambda_o)\ e^{-\frac{\sigma(a-x)}{\mu}} \tag{21}$$

The integration over x is performed analytically. The resultant distribution is then numerically integrated over θ, φ from the known Klein-Nishina cross-section.

A completely analogous procedure is used for higher k values. Thus $N_k(a,\lambda_o,\mu_o)$ is

$$N_k(a,\lambda_o,\mu_o) = \underbrace{\int_o^a \cdots \int_o^{a-\frac{\sigma x_i}{\mu}}}_{k \text{ terms}} \underbrace{\int \cdots \int}_{k \text{ terms}} d\Omega_i \sum_{i=0}^{k-1} e^{-\frac{\sigma_i x_i}{\mu_i}} \sigma_s(\theta,\lambda) *$$

$$* e^{-\frac{\sigma_i (a-x_i)}{\mu_i}} \tag{23}$$

In order to make the integrations over angle manageable it is assumed that only forward scattered photons contribute sensibly to the transmission. Consequently all the $\mu_i > 0$. Although the x integrations are analytic, the angular integrations are numeric. In particular 2k integrations are needed to evaluate N_k.

Because of the involved integrations usually the series are terminated at $k \leq 3$, and remaining values estimated. Without considering the details further, it is evident that the method has serious drawbacks for compact power plants. The relative merits are listed below.

Advantages:

1) Useful for quick surveys for thin shields.

2) Can be modified to yield energy transmission rather than number transmission.

3) The method has been extended to multi-layered shields.

Disadvantages:

1) Computational burden is large for large number of scattering components.

2) The results do not give all information desired, i.e., the spectrum and direction of emergent photons.

3) Other geometries are very difficult.

4) The errors are large for thick shields. In particular, it is difficult to even estimate the errors.

5) Although the method is actually an approximate solution of the integral transport equation, the approach is such that much useful information is not available, in distinction to the usual solution of the transport equation.

3.5 The Removal Cross Section Method

The simplest method of treating neutron penetration problems is the removal cross section method. The basis of the method is the observation that a neutron collision with hydrogen produces a lower energy neutron which does not penetrate much further due to the increasing hydrogen cross-section. Thus, the first collision density determines approximately the penetration properties of hydrogenous shields. For a sufficiently thick shield, the flux density should ultimately become exponential in nature.

The method is limited to neutrons from the fission spectrum. After a sufficient thickness of hydrogenous media (usually water) the lower energy neutrons are thermalized (and easily absorbed). The very high energy end of the spectrum is attenuated by the fission spectrum itself. The result is the spectrum "hardens" up to a certain thickness and then behaves roughly as a monoenergetic beam.

If a slab of material is introduced between the source and the hydrogenous medium, the behavior deep within the shield (i.e., the water) will be the same as without the slab but with reduced magnitude. Let $\varphi_o(x)$ be the hardened flux distribution in the absence of the slab, and $\varphi(x)$ the distribution with the slab. For sufficiently large x, it is phenomenologically true that

$$\varphi(x) = \alpha\varphi_o(x)$$

where α may be written $e^{-\sigma_r t}$, with t the slab thickness. The coefficient σ_r is the slab removal cross-section for the material and is independent of energy, x, and t.

The fact that such a simple approximation is valid depends crucially upon having a fission spectrum and a thick hydrogenous shield. The measurement of $\varphi(x)$ (or $\varphi_o(x)$) is actually very difficult and implicit in the removal cross-section measurement is the assumption that the thermal neutron flux parallels the fast flux for sufficiently large x.

The removal cross-section method can easily be extended to cover distributed shield material mixed with water. Although the method is very simple the actual physical measurement of σ_r for either slab or distributed shield material is rather difficult.

From this brief sketch, it is possible to rate the method.

Advantages:

1) Simple to use.

2) Can be very accurate under appropriate conditions.

3) Correction for irregularities in geometry, channels, piping, etc. are simple in this model.

Disadvantages:

1) Requires a thick hydrogeneous shield.

2) Lack of a theoretical model for predicting removal cross-section.

3) Uncertainties in cross-sections yield large uncertainties in penetration.

4.0 A PROPOSED SHIELD CALCULATION PROCEDURE

For all of the methods reviewed in Section 3.0, only the numerical integration of the transport equation gave all of the desired information regarding flux distributions. The major drawback with the method was the machine time required to obtain the desired information. If the calculational procedure could be reduced then the method would be the most general and most exact procedure available, save for analytic solutions.

The purpose of this section is to outline a new method of solution of boundary value problems which promises significant reduction in the time of calculation. The method has been applied successfully to diffusion calculations. The derivation of the technique will, therefore, be for diffusion calculations. A possible method of extension for transport problems is then discussed. It should be clearly understood that the proposed extension has not been attempted and hence constitutes a conjectured procedure.

For illustrative purposes the diffusion equation in the form

$$\nabla \cdot D(x,y)\ \nabla\varphi + \lambda^2 \rho(x,y)\ \varphi = 0 \tag{24}$$

is considered. The equation applies in the rectangular region $0 \leq x \leq a$, $0 \leq y \leq b$. A rectangular network is superimposed upon the region as shown in Figure 1.

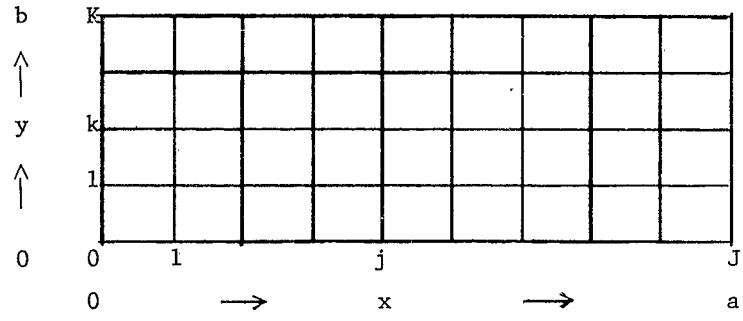


Figure 1

The Difference Mesh for the Rectangular Region $0 \leq x \leq a$; $0 \leq y \leq b$

The diffusion equation (24) is assumed to obey boundary conditions of the form

$$\begin{aligned} &\varphi(0,y) = f(y), \\ &\varphi(x,0) = \varphi(x,b) = 0 \\ &\varphi(a,y) = 0 \end{aligned} \tag{25}$$

The differential equation may be reduced to a difference equation of the form

$$a_{j,k}\,\varphi_{j+1,k} + b_{j,k}\,\varphi_{j,k} + c_{j,k}\,\varphi_{j-1,k} + d_{j,k}\,\varphi_{j,k-1} + e_{j,k}\,\varphi_{j,k+1} = 0 \tag{26}$$

Equation (26) applies of $0 < j < J$, $0 < k < K$, i.e., all interior points of the mesh. The boundary conditions for the finite difference equation become

$$\begin{aligned} &\varphi_{0,k} = f_k \\ &\varphi_{j,0} = \varphi_{j,K} = 0 \\ &\varphi_{J,k} = 0 \end{aligned} \tag{27}$$

The usual process for solving (26) is iterative. An assumed distribution, consistent with the boundary conditions, is iterated by the algorithm

$$\varphi^{p+1}_{j,k} = -\frac{1}{b_{j,k}}\left[a_{j,k}\varphi^{p}_{j+1,k} + c_{j,k}\varphi^{p}_{j-1,k} + d_{j,k}\varphi^{p}_{j,k-1} + e_{j,k}\varphi^{p}_{j,k+1}\right] \tag{28}$$

The superscript p denotes the iteration index. Other iterations are possible. Characteristically, iteration procedures such as (28) requires an amount of time proportional to $(JK)^2$.

The new method is based upon the following procedure. At the column $j = J-1$, define $\underline{\Psi}_{J-1}$ as

$$\underline{\Psi}_{J-1} = \begin{bmatrix} \varphi_{J-1,1} \\ \varphi_{J-1,2} \\ \vdots \\ \varphi_{J-1,K-1} \end{bmatrix}$$

Now choose K-1 different vectors $\underline{\psi}_{J-1}^{(n)}$ as follows

$$\underline{\psi}_{J-1}^{(n)} = \begin{bmatrix} \delta_{n,1} \\ \delta_{n,2} \\ \cdot \\ \cdot \\ \cdot \\ \delta_{n,K-1} \end{bmatrix} \tag{29}$$

Thus, the set $\underline{\psi}_{J-1}^{(n)}$ consists of the set of K-1 unit vectors and are complete in the space of dimension K-1. The basic difference relation (26) is factored in the form

$$\varphi_{j-1,k} = -\frac{1}{c_{j,k}}\left[a_{j,k}\varphi_{j+1,k} + b_{j,k}\varphi_{j,k} + d_{j,k}\varphi_{j,k-1} + e_{j,k}\varphi_{j,k+1}\right] \tag{30}$$

Then each vector $\underline{\psi}_{J-1}^{(n)}$ is extended, by equation (30), through the mesh to the column j = 0. Thus, K-1 vectors are generated at column 0, say $\underline{\psi}_{0}^{(n)}$. The set of vectors $\underline{\psi}_{0}^{(n)}$ is complete and hence the boundary condition f_j may be expanded as

$$f_j = \sum_n a_n \underline{\psi}_0^n \tag{31}$$

The same expansion for the vectors $\underline{\psi}_{j}^{(n)}$ then yields the desired solution. The entire procedure requires (K-1)(J-1) steps.

There are two objections to the method as it stands. First, the set $\underline{\psi}_{0}^{(n)}$ may not be complete and hence the expansion (31) is invalid. In general, this is indeed the case. The reason is that the march-out, equation (30) is unstable. That is, errors in the vectors $\underline{\psi}_{J-1}^{(n)}$ are amplified to such an extent that all $\underline{\psi}_{0}^{(n)}$ become proportional to one another irrespective of the value of $\underline{\psi}_{J-1}^{(n)}$. This follows since the eigenvalues of the march-out operator are greater than unity in general.

However, steps may be taken to prevent divergence of the march-out. In particular, if the set $\underline{\psi}_{j}^{(n)}$, which are orthogonal at j = J-1, are periodically orthogonalized, then the growing components are filtered and the completeness of the set is assured. The only exception is for λ^2 an eigenvalue of the equation, in which case no solution exists in any event. (Incidentally the method can therefore be used to solve eigenvalue problems also.)

The orthogonalization requires a number of steps proportional to $(K-1)^3$ and the entire procedure requires $(J-1)(K-1)^3$ steps. For particular problems there may be a significant reduction, i.e., when $J > K$. However, the method may still be improved.

The initial orthogonal set chosen was the unit vectors. Alternative sets may be used, for instance, the finite Fourier harmonics. If the solution is reasonably smooth only a few Fourier harmonics are necessary to specify the solution. Suppose the first M harmonics are sufficient. The number of steps, including the re-orthogonalization, is then $(K-1)(J-1)(M)^3$. The use of an incomplete set of harmonics introduces a truncation error. However, for most problems the amplitudes of the harmonics decreases rather rapidly on either side of the fundamental. Of course, other orthogonal vectors than the Fourier series are possible for use.

A practical procedure for selecting the number and range of vectors is to expand the boundary condition f_k and select only the significant vectors. Any desired order truncation error may be found.

All of the above ideas have been successfully applied to the diffusion equation. It has been found that the method permits a significant time saving for solution of the equation. In particular, the criticality problem has been solved for the first 5 critical eigenvalues with ease, a problem that is very difficult by other means. The use of a truncated orthogonal series has been used to solve inhomogeneous problems and experimentally it is found that 3 vectors are sufficient to reduce the truncation error to below 1/2%. Further research is needed to find more general rules for selecting the proper vectors.

The application of the method to the transport equation is not as clear cut as the above. The particular problem of concern is the boundary conditions. Consider a finite mesh in x-μ spare as shown in Figure 2.

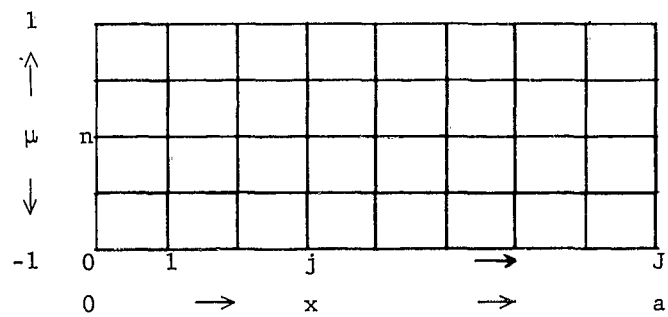


Figure 2

A Discrete Mesh in r-μ Spare for the 1 Group Transport Equation

The appropriate boundary conditions at $x = 0$ include the incident current, i.e., $\mu > 0$. However, nothing is known about the emergent current, i.e., $\mu < 0$. Likewise at $x = a$, the incident current is zero for a vacuum interface. This specifies $\varphi(a,\mu)$, $\mu < 0$. Again, nothing is known about the flux for $\mu > 0$, that is the leakage. The boundary condition at $\mu = \pm 1$ for all x are merely $\frac{\partial \varphi}{\partial \mu} = 0$, that is no gradient of the directional flux.

One possible approach is to consider the flux density to vanish at the extrapolated end point of the region at $x = a$. For shielding studies it is not clear that such an approximation is proper, since the exit current is precisely the desired information. Furthermore, for different energy groups, the end-point is variable.

An alternative procedure is to divide the mesh at $\mu = 0$ into two problems with the condition that $\varphi(x,0)$ be continuous. The difficulty here is the treatment of the line at $\mu = 0$. Further, the expansion vectors along the portion of the problem for $\mu > 0$ need not be the same for $\mu < 0$.

It is clear from the above discussion that some effort should be expended in adopting the procedure to transport problems. The promise of the reduction in time justifies considerable effort in this direction.

Under the assumption that the method can be adopted to the transport equation, the numerical solution would then be the preferred method of attack for compact power reactor shields. For the very difficult geometries such as rocket vehicles, the numerical integration solution over the primary shield must be coupled with another method for solving for scattered radiation into the payload. Monte Carlo is at present the only reasonable procedure.

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Rpt. No. ESD-TDR-63-231. TECHNIQUES FOR NUCLEAR SHIELDING CALCULATIONS. Final report, May 1963, 33p incl. illus., 12 refs.
Unclassified Report

Reviews and critiques of selected methods for nuclear shielding calculations are presented. Those techniques considered are numerical integration of the Boltzmann equation,

1. Nuclear power plants
2. Radiation damage
3. Equations
I. Project No. 477
II. Contract AF19 (628)-2390
III. The MITRE Corporation, Bedford, Mass.
IV. Hansen, K.F.
V. TM-3522

moments method, Monte Carlo, method of successive scatterings, and removal cross-section method. An outline of the advantages and disadvantages of each particular method is included, along with a new simplified calculation procedure.	VI. In ASTIA collection	moments method, Monte Carlo, method of successive scatterings, and removal cross-section method. An outline of the advantages and disadvantages of each particular method is included, along with a new simplified calculation procedure.	VI. In ASTIA collection
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